

Self-consistent theory of intrinsic localized modes: application to monatomic chain

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Abstract

A theory of intrinsic localized modes (ILMs) in anharmonic lattices is developed, which allows one to reduce the original nonlinear problem to a linear problem of small variations of the mode. This enables us to apply the Lifshitz method of the perturbed phonon dynamics for the calculations of ILMs. In order to check the theory, the ILMs in monatomic chain are considered. A comparison of the results with the corresponding molecular dynamics calculations shows an excellent agreement.

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Key words: Lattice vibrations; Anharmonicity; Intrinsic localized mode.

1 Introduction

It is already a well-known fact that localized vibrational excitations can exist in perfect anharmonic lattices [1,2,3,4,5,6,7,8,9,10]. Such excitations are called intrinsic localized modes (ILMs) [4], discrete breathers [8] or discrete solitons [10]. The main approach, which has been used for the study of these vibrational excitations so far, is molecular dynamics (MD) simulations, which are based on the numerical integration of the classical equations of motion in a lattices with a finite number of the degrees of freedom. The approach is rather efficient in the case of simple 1D lattices (see, e.g. [11,12,13,14,15,16,17,18,19,20,21,22]), but requires very lengthy computations in the case of 2D and 3D lattices due to the rapid growth of the number of numerical operations with the increase of the number of the vibrational degrees of freedom (see [23,24,25]). Therefore, it is of interest to develop other methods which would allow one, when studying ILMs, to reduce the amount of numerical computations.

Below we are developing a mean-field-type theory of ILMs which allows one to perform calculations for macroscopically large lattices of arbitrary dimensions. The theory is based on the consideration of small variations of the ILM amplitude. The equations for these variations include characteristics of the ILM. This allows us to reduce the nonlinear problem of the ILM to a linear problem of the perturbed phonon dynamics; the perturbation comes from the ILM and it is determined self-consistently. To describe the effect of the perturbation we apply the Greens' function method of the perturbed local dynamics of phonons (the Lifshitz method), allowing us to calculate the ILM. As compared to the method [4], which also uses the Greens functions of the perfect harmonic lattice for calculations of strongly localized ILMs, our method works generally, including the cases when ILMs have remarkable size. To test the theory, we consider the even and odd ILMs in a monatomic chain. In parallel, the molecular dynamics simulations of these ILMs are carried out. The comparison of the results of both calculations shows an excellent agreement.

2 Self-consistency equations

Let us start with the classical equations of the motion of atoms in a lattice

$$M_n \ddot{u}_n = - \sum_k \sum_{n_1 n_2 \dots} V_{nn_1 \dots n_{k-1}}^{(k)} u_{n_1} u_{n_2} \dots u_{n_{k-1}}. \quad (1)$$

Here u_n is the Cartesian displacement of the atom n , M_n is its mass, $V^{(2)}$, $V^{(3)}$, \dots are the harmonic and anharmonic springs; the subscripts n include both the site number and the number of the Cartesian component. We are considering a localized solution of the equation (1) describing the stable ILM. The corresponding displacements of atoms are of the form

$$u_n(t) = \xi_n + A_n \cos \omega_l t + O(\omega_l),$$

where ω_l is the frequency of the ILM which lies outside the phonon spectrum, $|A_n|$ is the amplitude of the ILM at the site n , ξ_n is the shift of the equilibrium position of the atom n (i.e. the dc-component of the ILM; this component differs from zero due to odd anharmonicities), $O(\omega_l)$ is the sum of the higher harmonics. The contributions of these harmonics are usually rather small [3,4,5,6,7,8,9]. Below they will be neglected.

In our further consideration, we shall make use of the fact that $u_n(t + \tau)$ is also a periodic solution of the equation (1). Taking τ to be infinitesimal, we can find small variation of the ILM $q_n(t) = u_n(t + \tau) - u_n(t) = -A_n \tau \sin \omega_l t$,

which also oscillate in time with the frequency ω_l and amplitudes $\sim A_n$ (note the phase shift $\pi/2$ of $q_n(t)$); it satisfies the equation:

$$M_n \ddot{q}_n = - \sum_{n'} (V_{nn'}^{(2)} + \partial^2 V_{\text{anh}} / \partial u_n \partial u_{n'}) q_{n'}, \quad (2)$$

where V_{anh} is the anharmonic part of the potential energy. We consider the $\propto \sin \omega_l t$ terms of this equation (i.e. we neglect higher-order harmonics of it). Taking into account that the $\propto \sin \omega_l t$ term of the product $\cos^{2n} \omega_l t \sin \omega_l t$ coincides with the time-independent term of the product $2 \cos^{2n} \omega_l t \sin^2 \omega_l t$, we get

$$M_n \ddot{q}_n = - \sum_{n'} (V_{nn'}^{(2)} + v_{nn'}) q_{n'}, \quad (3)$$

where

$$v_{nn'} = 2 \langle \sin^2 \omega_l t \partial^2 V_{\text{anh}} / \partial u_n \partial u_{n'} \rangle. \quad (4)$$

Here the partial derivative is taken for $u_n = \xi_n + A_n \cos \omega_l t$,

$$\langle \dots \rangle = \frac{\omega_l}{2\pi} \int_0^{2\pi/\omega_l} \dots dt$$

denotes the averaging over the period $2\pi/\omega_l$.

The dc-shifts ξ_n are not the independent parameters of the problem: they are determined by the ILM amplitudes. The corresponding relation reads [26]

$$\xi_n = \sum_{n'} g_{nn'} \langle \partial V_{\text{anh}} / \partial u_{n'} \rangle, \quad (5)$$

where $g_{nn'} = G_{nn'}^{(0)}(0) / \sqrt{M_n M_{n'}}$, $G_{nn'}^{(0)}(0)$ is the static limit ($\omega = 0$) of the Green's function of the perfect lattice [27,28]

$$G_{nn'}^{(0)}(\omega) = \sum_j e_{nj} e_{n'j} / (\omega^2 - \omega_j^2),$$

$e_{nj} \propto e^{ik_j n}$ is the polarization vector of the phonon j , k_j is its wave vector.

Our further consideration is based on the observation that the equation (3) corresponds to the following harmonic potential energy

$$V_{\text{MF}} = \frac{1}{2} \sum_{nn'} (V_{nn'}^{(2)} + v_{nn'}) q_n q_{n'}. \quad (6)$$

This potential energy, if the amplitude parameters A_n are chosen correctly, should lead to the appearance of the linear local mode, being an infinitesimal part of the ILM. The potential V_{MF} constitutes a mean field for the linear mode and, therefore for the ILM. The matrix $v_{nn'}$ gives the required change of the elastic springs.

The potential V_{MF} should be determined self-consistently. This can be done by applying the Lifshitz method [27] of the local dynamics in harmonic approximation. In this method, the amplitude parameters satisfy the relations

$$A_n/A_0 = G_{n0}(\omega_l)/G_{00}(\omega_l), \quad (7)$$

where $G(\omega)$ is the matrix of the perturbed Green's function being equal [27]

$$G(\omega) = (I - G^{(0)}(\omega) v)^{-1} G^{(0)}(\omega), \quad (8)$$

the frequency ω_l is given by the position of the pole of $G(\omega)$ outside the phonon spectrum. Taking into account that the amplitude parameters A_n enter into the perturbation matrix v , one can conclude that equations (7) together with the pole condition $(I - G^{(0)}(\omega) v)^{-1} \rightarrow \infty$ constitute the self-consistency equations.

To calculate an ILM by means of the proposed method, one should choose the main amplitude(s) of the ILM and to fix a possible values of few other amplitudes. Using these amplitudes one can find the dc-shifts ξ_n by solving the equation (5). Inserting obtained ξ_n into Eq. (4) one can calculate matrix v . After that one should calculate the frequency of the ILM and the relative amplitudes, using equations (8) and (7). If the obtained A_n differ from the chosen initially, the calculations should be repeated with newly found amplitudes.

The presented theory can be applied for different, including 3D, anharmonic lattices.

3 Test for monatomic chain

As a test of the presented theory we consider the well-known case of ILMs in a monatomic chain, taking into account only the nearest-neighbor interactions and the positive quartic anharmonicity. The potential energy of vibrations in this case has the form

$$V = \frac{1}{2} \sum_n \bar{u}_n^2 \left[K_2 + \frac{1}{2} K_4 \bar{u}_n^2 \right], \quad (9)$$

where $\bar{u}_n = u_n - u_{n-1}$ is the difference of the shifts of the particles n and $n - 1$. The top phonon frequency equals $\omega_m = 2\sqrt{K_2}$. In our calculations we took $K_2 = 100$ which corresponds to $\omega_m = 20$. The Green's functions of the harmonic chain equal [28]

$$G_{nn'}^{(0)}(\omega) = [-\rho(\omega)]^{|n-n'|} / \omega \sqrt{\omega^2 - 1}, \quad (10)$$

where $\rho(\omega) = (\omega - \sqrt{\omega^2 - 1})^2 \leq 1$ (in Eq. (10) the units $\omega_m = M = 1$ are used).

The dc-shifts in this model equal zero, and the equation for the perturbation matrix v can be found straightforward:

$$v_{nn'} = \delta_{n,n'}(\gamma_{n+1} + \gamma_n) - \delta_{n-1,n'}\gamma_n - \delta_{n+1,n'}\gamma_{n+1}. \quad (11)$$

Here

$$\gamma_n = \frac{3}{4} K_4 \bar{A}_n^2 \quad (12)$$

is the renormalization of the elastic spring between the atoms n and $n - 1$, $\bar{A}_n = A_n - A_{n-1}$. For $K_4 > 0$ all γ_n are positive. Therefore the ILMs appear above the phonon spectrum; they have an odd or an even symmetry.

First we study an even ILM centered at the atoms $n = 0$ and $n = -1$. In this case, the amplitude parameters satisfy the condition $A_{n-1} = -A_n$. We consider only ILMs which have the largest amplitude on the atoms $n = 0$ and $n = -1$ and take into account the contributions of 8 central atoms. In this case we include into consideration the renormalization of 7 central springs given by γ_0 , $\gamma_{\pm 1}$, $\gamma_{\pm 2}$ and $\gamma_{\pm 3}$ (see Eq. (12)). These parameters can be determined together with the frequency and the amplitudes self-consistently using the equations (8) and (7). The latter we treat iteratively: we start with the amplitude ratios given in [5] and then find the frequency, the values of the

amplitudes and then their corrections from these equations and so on. The iteration procedure converges fast. The results of the calculations can be seen in Table 1 and in Fig. 1 (theory).

Now we consider an odd ILM centered at the $n = 0$ atom. Then the amplitude parameters of the ILMs satisfy the condition $A_n = A_{-n}$. We restrict ourself with consideration only of ILMs having the largest amplitude on the central atom, and take into account the contribution of 7 central atoms. In this case we take into account the changes by the ILMs of 6 central springs given by γ_0 , $\gamma_{\pm 1}$, $\gamma_{\pm 2}$ and γ_3 (see Eq. (12)). As in the case of even ILMs, the springs parameters are determined together with the frequency and the amplitudes self-consistently using the equations (8) and (7). The results of the calculations can be seen in Fig. 1 (theory) and in Table 1.

4 Comparison with MD calculations

In the case under consideration, one can easily find the ILMs numerically by integrating the equations of motion. In our calculations we used the forth-order Runge-Kutta algorithm. The results of calculations are compared with the theory. In Fig. 1 and in Table 1 one can see that the theoretical and the MD calculations of the ILMs frequencies and amplitudes are in very good agreement.

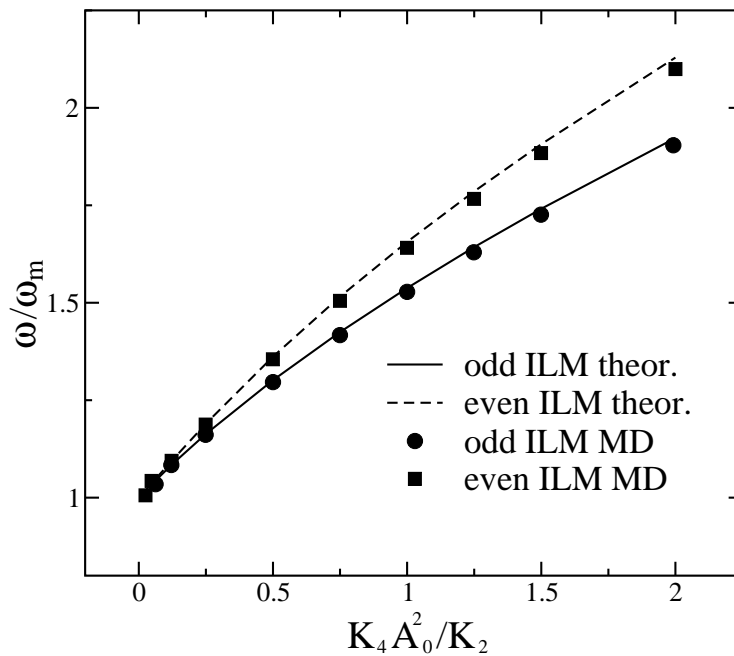


Fig. 1. Frequency dependences of the intrinsic localized modes in a monatomic chain with a hard quartic anharmonicity versus the dimensionless anharmonicity parameter $K_4 A_0^2 / 4K_2$; $|A_0|$ is the ILM amplitude on the central atom.

Table 1

Frequencies and amplitudes of the even and odd ILMs in a monatomic chain with a hard quartic anharmonicity. For every K_4 two values of the parameters mentioned are given: the theoretical value (up) and the result of the MD calculation (down).

Even ILM						
K_4	$\frac{K_4}{K_2}A_0^2$	$\frac{\omega_l}{\omega_m}$	A_0	$-A_1$	A_2	$-A_3$
50	0.1250	1.0963	0.5000	0.3211	0.1537	0.0662
	0.1224	1.0945	0.4947	0.3208	0.1550	0.0680
200	0.5000	1.3617	0.5000	0.1981	0.0419	0.0084
	0.4996	1.3551	0.4998	0.1981	0.0421	0.0083
800	2.0000	2.1289	0.5000	0.1218	0.0084	0.0005
	1.9999	2.0995	0.4999	0.1219	0.0085	0.0005
Odd ILM						
K_4	$\frac{K_4}{K_2}A_0^2$	$\frac{\omega_l}{\omega_m}$	A_0	$-A_1$	A_2	$-A_3$
50	0.1250	1.0862	0.5000	0.4034	0.2266	0.1054
	0.1210	1.0839	0.4920	0.3989	0.2288	0.1117
200	0.5000	1.3014	0.5000	0.3315	0.0999	0.0225
	0.4998	1.2965	0.4999	0.3314	0.1001	0.0229
800	2.0000	1.9228	0.5000	0.2858	0.0386	0.0031
	1.9920	1.9040	0.4990	0.2726	0.0358	0.0029

Note that the small discrepancies between the theoretical and the MD values of the ILM frequency ω_l increases with ω_l . The reason is that we have neglected the higher harmonics: the contribution of these harmonics to an ILM is the larger the larger is the frequency.

5 Conclusion

To conclude, we have developed a theory of intrinsic localized modes in anharmonic lattices, which allows one to make use of harmonic approximation results and to perform calculations for a macroscopically large lattice. We have derived the equations describing small variations of ILMs amplitudes, which allowed us to reduce the original nonlinear problem to the linear problem of phonon localization on the local effective potential. The latter is created by the ILM itself and it is determined self-consistently. This enabled us to apply the Greens' function method of the perturbed local dynamics of phonons (the Lifshitz method) for the calculations of ILMs. The theory works generally,

including the cases when ILMs have remarkable size. To test the theory we calculated even and odd ILMs in an anharmonic monatomic chain. We have also carried out the MD calculations of the ILMs in the chain. A comparison of the results, obtained by both methods (see Fig. 1 and Table 1) gives full confirmation of the proposed theory. Although concrete calculations here are performed only for the monatomic chain, the theory itself is general and can be applied for different lattices, including 3D crystals with arbitrary anharmonic potentials.

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